Spectroscopic Observation of Binary (Cyclopropanemethanol + Methane) Hydrates

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Here, new structure II (sII) hydrate with cyclopropanemethanol (CPM) in the presence of methane (CH₄) are investigated for the first time through spectroscopic tools, such as solid-state NMR, high-resolution powder X-ray diffraction, and Raman spectroscopy. Solid-sate NMR spectroscopy is used to describe the crystal structure and guest distributions of binary CPM + CH₄ hydrate, and we confirm the formation of sII hydrate with CPM in the presence of CH₄. The inclusion of CH₄ gas in the both large and small cages of sII hydrate are also identified by Raman spectroscopy. In addition, we also analyze the inclusion behaviors of CPM in the large cages of sII hydrate, and there is no existence of free OH signal from Raman spectra of binary CPM + CH₄ hydrate. HRPD pattern of binary CPM + CH₄ hydrate is analyzed by Rietveld analysis with direct space method, and we reveal that hydroxyl group of CPM may have strong hydrogen bonding ability with the host water molecules. Finally, we also measure the phase equilibrium conditions of binary CPM + CH₄ hydrate.

KEYWORDS gas hydrate, cyclopropanemethanol, methane, Raman, phase equilibrium